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Software concepts for coupling reduced and detailed simulations

Workshop on Reduced Basis Methods, Ulm

wissen.leben WWU Münster

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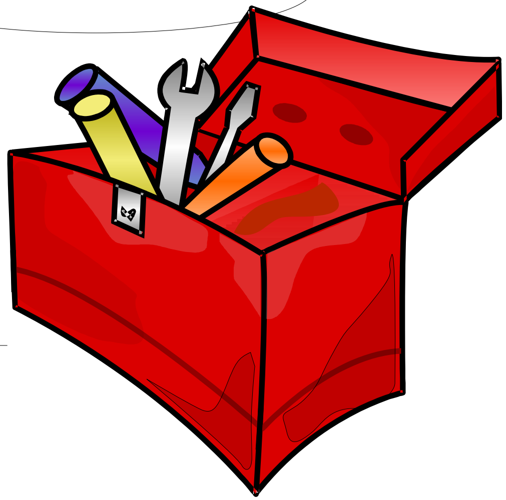
> Motivation

PDE Discretizations (FEM, FV, DG):
Navier-Stokes, Groundwater-Flow, Convection-Diffusion,
Poisson, Maxwell, ...

Parametrization



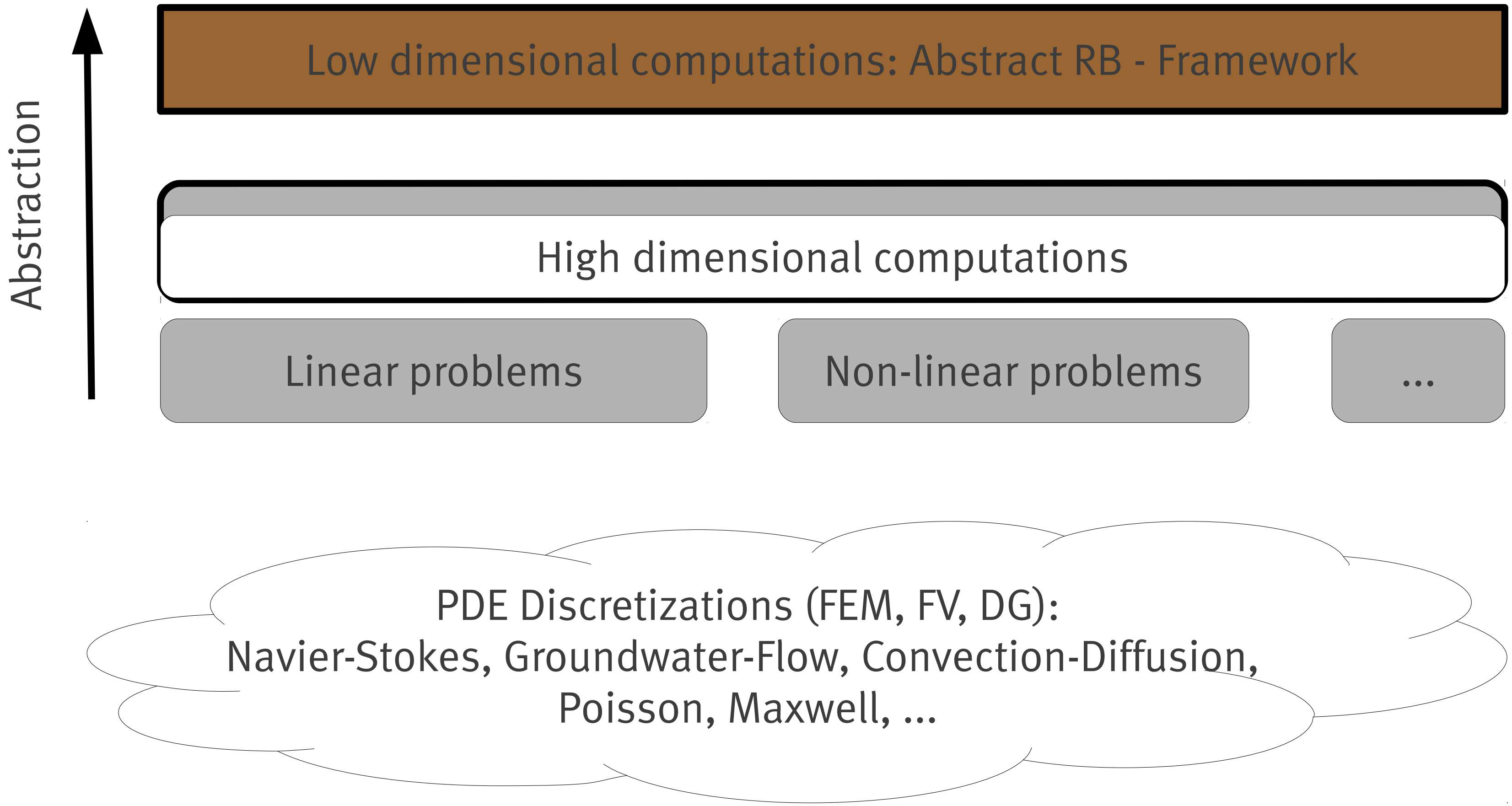
Magical RB-Tools

Reduced model

› Goals Specification

- Abstract Reduced Basis Framework
- Re-use of (existing) efficient implementations of PDE discretizations
- Short time for implementing the detailed simulations as reduced simulations

› Abstract Software Concept



› Low dimensional Computations (RBMATLAB)

- Control of Offline-Algorithms
  - POD-Greedy Algorithm, Empirical Interpolation Algorithm
  - Gathering and post-processing of reduced matrices
- Low-Dimensional Computations
  - Reduced Simulations
  - A posteriori error estimation
- Low dimensional data visualization
- (Implemented in MATLAB)

High dimensional computations (DUNE-RB)

- Storage / Manipulation of reduced spaces
- Efficient high dimensional linear algebra algorithms
  - POD, Orthonormalization, Gram-Matrix computations
- Parametrization
- (Implemented in C++, based on
  - DUNE core modules (http://dune-project.org) and
  - DUNE-FEM (dune.mathematik.uni-freiburg.de)

The Glue

- Communication between DUNE-RB and RBMATLAB can be realized by

    1. compiling DUNE-RB as (mex-) library for matlab or:
    2. TCP/IP Communication between two stand-alone applications

Proof of Concept (linear evolution problem)

```
RBMATLAB > matlab

                  < M A T L A B (R) >
        Copyright 1984-2008 The MathWorks, Inc.
              Version 7.6.0.324 (R2008a)
                   February 10, 2008


  To get started, type one of these: helpwin, helpdesk, or demo
.
  For product information, visit www.mathworks.com.

starting up rbmatlab in directory:
/home/martin/projects/rbm-results/rbmatlab
Using the following directory for large temporary data:
/tmp
Using the following directory for data files storing results:
/home/martin/projects/rbm-results/results
Using the following directory as RBMATLABHOME:
/home/martin/projects/rbm-results/rbmatlab
skipped clearing filecache for function-calls!
>>
```

```
DUNE-RB > ./dunerbServer
YaspGridParameterBlock: Parameter 'overlap' not specified, defa
ulting to '0'.
server: waiting for connections...
```

Proof of Concept (linear evolution problem)

```
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Using the following directory as RBMATLABHOME:
/home/martin/projects/rbm-results/rbmatlab
skipped clearing filecache for function-calls!
>>
>> [a,b,c] = ...
mexclient('echo', [1, 2], ....
                  struct('field', [1,2]), ...
                  { [1,2], [3,4] });
client: connect: Connection refused
Warning: connection to ::1 failed

client connected to 127.0.0.1
copying argument no. 0
copying argument no. 1
copying argument no. 2
>>
```

```
DUNE-RB > ./dunerbServer
YaspGridParameterBlock: Parameter 'overlap' not specified, defa
ulting to '0'.
server: waiting for connections...
server: got connection from 127.0.0.1

Received call for processing 'echo'
with 4 arguments and 3 return values.
=======================================================

copying argument no. 0
copying argument no. 1
copying argument no. 2
```

Proof of Concept (linear evolution problem)

```
/home/martin/projects/rbm-results/rbmatlab
skipped clearing filecache for function-calls!
>>
>> [a,b,c] = ...
mexclient('echo', [1, 2], ....
                  struct('field', [1,2]), ...
                  { [1,2], [3,4] });
client: connect: Connection refused
Warning: connection to ::1 failed

client connected to 127.0.0.1
copying argument no. 0
copying argument no. 1
copying argument no. 2
>> a

a =

     1     2

>> b

b =

    field: [1 2]

>> c

c =

    [1x2 double]    [1x2 double]

>>
```

```
DUNE-RB > ./dunerbServer
YaspGridParameterBlock: Parameter 'overlap' not specified, defa
ulting to '0'.
server: waiting for connections...
server: got connection from 127.0.0.1

Received call for processing 'echo'
with 4 arguments and 3 return values.
======================================================

copying argument no. 0
copying argument no. 1
copying argument no. 2
```

Proof of Concept (linear evolution problem)

```
                    < M A T L A B (R) >
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Using the following directory for data files storing results:
/home/martin/projects/rbm-results/results
Using the following directory as RBMATLABHOME:
/home/martin/projects/rbm-results/rbmatlab
skipped clearing filecache for function-calls!
>>
>>
>> % load model parameters
>>
>> model = convdiff_dune_model;
Warning: Name is nonexistent or not a directory: mexclient.
> In path at 110
  In addpath at 87
  In convdiff_dune_model at 95
client: connect: Connection refused
Warning: connection to ::1 failed

client connected to 127.0.0.1
>>
```

```
DUNE-RB > ./dunerbServer
YaspGridParameterBlock: Parameter 'overlap' not specified, defa
ulting to '0'.
server: waiting for connections...
server: got connection from 127.0.0.1

Received call for processing 'init_model'
with 1 arguments and 1 return values.
=======================================================

read discfunclist_xdr from headerfile, size = 20
Using the explicit ode solver! In order to use a different disc
retization, change the 'DISCRETIZATION' make variable

Received call for processing 'get_mu'
with 1 arguments and 1 return values.
=======================================================


Received call for processing 'rb_symbolic_coefficients'
with 1 arguments and 1 return values.
=======================================================
```

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Proof of Concept (linear evolution problem)

```
> In path at 110
  In addpath at 87
  In convdiff_dune_model at 95
client: connect: Connection refused
Warning: connection to ::1 failed

client connected to 127.0.0.1
>>
>> model.rb_problem_type

ans =

lin_evol
>> model.RB_generation_mode

ans =

greedy_uniform_fixed
>> model.RB_stop_Nmax

ans =

    20
>> model.T                        % this is read from DUNE-RB <<<<<<

ans =

     1

>>
```

```
DUNE-RB > ./dunerbServer
YaspGridParameterBlock: Parameter 'overlap' not specified, defa
ulting to '0'.
server: waiting for connections...
server: got connection from 127.0.0.1

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Proof of Concept (linear evolution problem)

```
ans =

lin_evol

>> model.RB_generation_mode

ans =

greedy_uniform_fixed

>> model.RB_stop_Nmax

ans =

    20

>> model.T                   % this is read from DUNE-RB <<<<<<

ans =

     1

>>
>>
>>
>>
>> % generate high dimensional model specific data, like e.g.
>> % the grid
>>
>> model_data = gen_model_data(model);
>>
>>
```

```
DUNE-RB > ./dunerbServer
YaspGridParameterBlock: Parameter 'overlap' not specified, defa
ulting to '0'.
server: waiting for connections...
server: got connection from 127.0.0.1

Received call for processing 'init_model'
with 1 arguments and 1 return values.
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read discfunclist_xdr from headerfile, size = 20
Using the explicit ode solver! In order to use a different disc
retization, change the 'DISCRETIZATION' make variable

Received call for processing 'get_mu'
with 1 arguments and 1 return values.
=======================================================


Received call for processing 'rb_symbolic_coefficients'
with 1 arguments and 1 return values.
=======================================================


Received call for processing 'gen_model_data'
with 1 arguments and 1 return values.
=======================================================
```

Proof of Concept (linear evolution problem)

```
>> % Just for fun: Do a DETAILED simulation in DUNE-RB >>>>>>
>>
>> %   first set the parameter mu
>> model = set_mu(model, [0.0 0.5 1.0]);
>>
>> %   then run the simulation
>> tic; sim_data = detailed_simulation(model, model_data); toc
Elapsed time is 11.795319 seconds.
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```

```
Received call for processing 'rb_symbolic_coefficients'
with 1 arguments and 1 return values.
=============================================================


Received call for processing 'gen_model_data'
with 1 arguments and 1 return values.
=============================================================


Received call for processing 'set_mu'
with 2 arguments and 0 return values.
=============================================================


Received call for processing 'detailed_simulation'
with 1 arguments and 1 return values.
=============================================================

opening file: ./grape//solution.series

Received call for processing 'set_mu'
with 2 arguments and 0 return values.
=============================================================


Received call for processing 'detailed_simulation'
with 1 arguments and 1 return values.
=============================================================

opening file: ./grape//solution.series
```

Proof of Concept (linear evolution problem)

```
>> % Just for fun: Do a DETAILED simulation in DUNE-RB >>>>>>
>>
>> %   first set the parameter mu
>> model = set_mu(model, [0.0 0.5 1.0]);
>>
>> %   then run the simulation
>> tic; sim_data = detailed_simulation(model, model_data); toc
Elapsed time is 11.795319 seconds.
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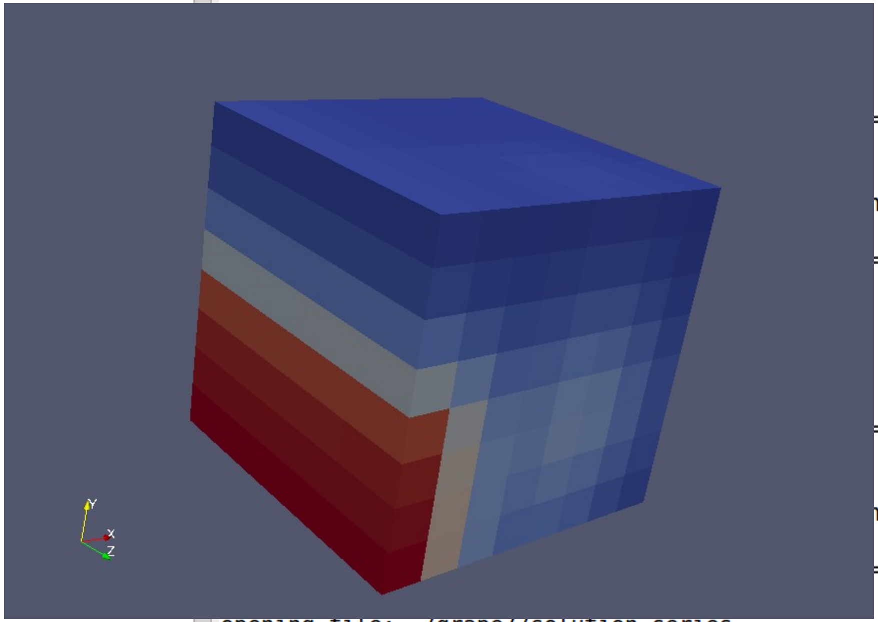
```

11.8 seconds!

```
Received call for processing 'rb_symbolic_coefficients'
with 1 arguments and 1 return values.
===========================================================

Received call for processing 'gen_model_data'
with 1 arguments and 1 return values.
===========================================================
opening file: ./grape//solution.series
```



Proof of Concept (linear evolution problem)

```
>> % Generate the reduced basis with the POD-Greedy algorithm
>> % in DUNE-RB >>>>>>>>
>>
>> detailed_data = gen_detailed_data(model, model_data);
Starting RB extension loop

Detected maximum error prediction 0.044006 for mu=[0.001
    1         0.5]
Extended RB to length 2

Detected maximum error prediction 0.015456 for mu=[0  1
Extended RB to length 3

Detected maximum error prediction 0.012877 for mu=[0
1         0.5]
Extended RB to length 4

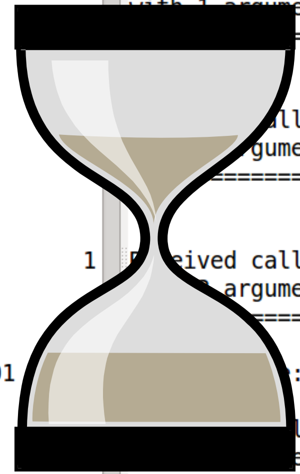
Detected maximum error prediction 0.01064 for mu=[0          1
         0.5]
Extended RB to length 5

Detected maximum error prediction 0.0084073 for mu=[0.001
   0.5          1]
Extended RB to length 6

Detected maximum error prediction 0.0073233 for mu=[0  1  1]
Extended RB to length 7

Detected maximum error prediction 0.0055443 for mu=[0  1  1]
Extended RB to length 8

Detected maximum error prediction 0.0048443 for mu=[0
 1         0.5]
```



```
Received call for processing 'rb_operators'
with 2 arguments and 1 return values.
======================================================

Received call for processing 'get_mu'
with 1 arguments and 1 return values.
======================================================

    ll for processing 'set_mu'
    guments and 0 return values.
======================================================

  eived call for processing 'rb_extension_PCA'
   arguments and 1 return values.
======================================================

       : ./grape//solution.series

      l for processing 'set_mu'
      ents and 0 return values.
======================================================

Received call for processing 'rb_init_values'
with 2 arguments and 1 return values.
======================================================
```

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Proof of Concept (linear evolution problem)

```
>>
>>
>> detailed_data.RB_info

ans =

                      M_train: [3x64 double]
             max_err_sequence: [1x20 double]
                  mu_sequence: [3x20 double]
                   mu_ind_seq: [1x20 double]
           toc_value_sequence: [1x20 double]
                 M_first_errs: [64x1 double]
           stopped_on_epsilon: 0
    stopped_on_max_val_train_ratio: 0
           stopped_on_timeout: 0
              stopped_on_Nmax: 1
       stopped_on_empty_extension: 0
     stopped_on_Nlimit_estimation: 0
                  M_last_errs: [64x1 double]
                 elapsed_time: 3.0000e-06

>>
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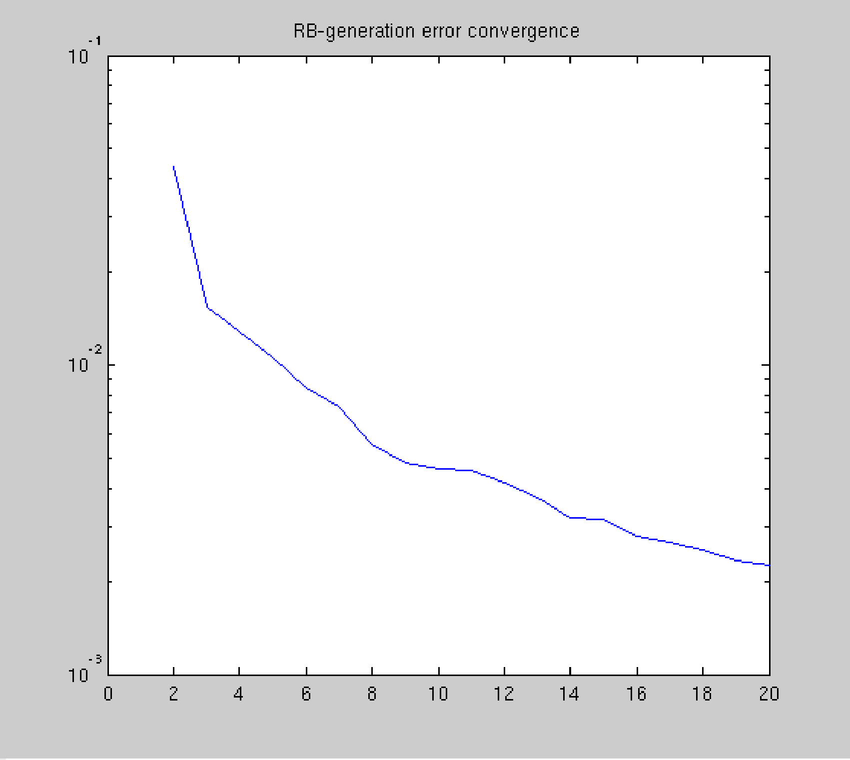
```

```
Received call for processing 'is_valid_rb'
```




```
opening file: ./grape//solution.series
```

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Proof of Concept (linear evolution problem)

```
>> % NOW: Generate reduced matrices for online computations
>> % and get them to RBMATLAB <<<<<<<<
>>
>> reduced_data = gen_reduced_data(model, detailed_data)

reduced_data =

      a0: {[1x20 double]}
    LL_I: {2x1 cell}
    LL_E: {5x1 cell}
      bb: {4x1 cell}
    K_II: {4x1 cell}
    K_IE: {10x1 cell}
    K_EE: {25x1 cell}
     m_I: {8x1 cell}
     m_E: {20x1 cell}
       m: {16x1 cell}
       N: 20

>>
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```

```
Received call for processing 'rb_init_values'
with 2 arguments and 1 return values.
======================================================


Received call for processing 'rb_operators'
with 2 arguments and 1 return values.
======================================================


Received call for processing 'set_mu'
with 2 arguments and 0 return values.
======================================================


Received call for processing 'reconstruct_and_compare'
with 2 arguments and 0 return values.
======================================================

opening file: ./grape//solution.series

Received call for processing 'rb_init_values'
with 2 arguments and 1 return values.
======================================================


Received call for processing 'rb_operators'
with 2 arguments and 1 return values.
======================================================
```

Proof of Concept (linear evolution problem)

```
>> % The matrices are all of small sizes: e.g. the explicit
>> % discretization operator: LL_E
>>
>> sizes=cellfun(@(X) size(X), reduced_data.LL_E, ...
                               'UniformOutput', false);
>> sizes{:}

ans =

    20    20


ans =

    20    20


ans =

    20    20


ans =

    20    20


ans =

    20    20

>>
>>
```

```
Received call for processing 'rb_init_values'
with 2 arguments and 1 return values.
=====================================================


Received call for processing 'rb_operators'
with 2 arguments and 1 return values.
=====================================================


Received call for processing 'set_mu'
with 2 arguments and 0 return values.
=====================================================


Received call for processing 'reconstruct_and_compare'
with 2 arguments and 0 return values.
=====================================================

opening file: ./grape//solution.series

Received call for processing 'rb_init_values'
with 2 arguments and 1 return values.
=====================================================


Received call for processing 'rb_operators'
with 2 arguments and 1 return values.
=====================================================
```

Proof of Concept (linear evolution problem)

```
>> % Now fast reduced simulations are possible in RBMATLAB
>> % without any communication to DUNE-RB
>>
>> model = model.set_mu(model, [0 0.5 1], true);
>>
>> tic; rb_sim_data=rb_simulation(model, reduced_data); toc
Elapsed time is 0.020223 seconds.
>>
>>
>> rb_sim_data

rb_sim_data =

        a: [20x113 double]
    Delta: [1x113 double]
     LL_I: [20x20 double]
     LL_E: [20x20 double]

>>
>>
>> % Error estimator at end time:
>>
>> rb_sim_data.Delta(end)

ans =

    0.0019

>>
>>
>>
>>
>>
```

0.02 seconds!

```
Received call for processing 'rb_init_values'
with 2 arguments and 1 return values.
======================================================

Received call for processing 'rb_operators'
with 2 arguments and 1 return values.
======================================================

Received call for processing 'set_mu'
with 2 arguments and 0 return values.
======================================================

Received call for processing 'reconstruct_and_compare'
with 2 arguments and 0 return values.
======================================================

opening file: ./grape//solution.series

Received call for processing 'rb_init_values
with 2 arguments and 1 return values.
======================================================

Received call for processing 'rb_operators'
with 2 arguments and 1 return values.
======================================================
```

Proof of Concept (linear evolution problem)

```
>> % Of course, the solution can be reconstructed in
>> % DUNE-RB >>>>>>>>>
>>
>> tic;...
dummy=rb_reconstruction(model, detailed_data, rb_sim_data); toc
Elapsed time is 0.359108 seconds.
>>
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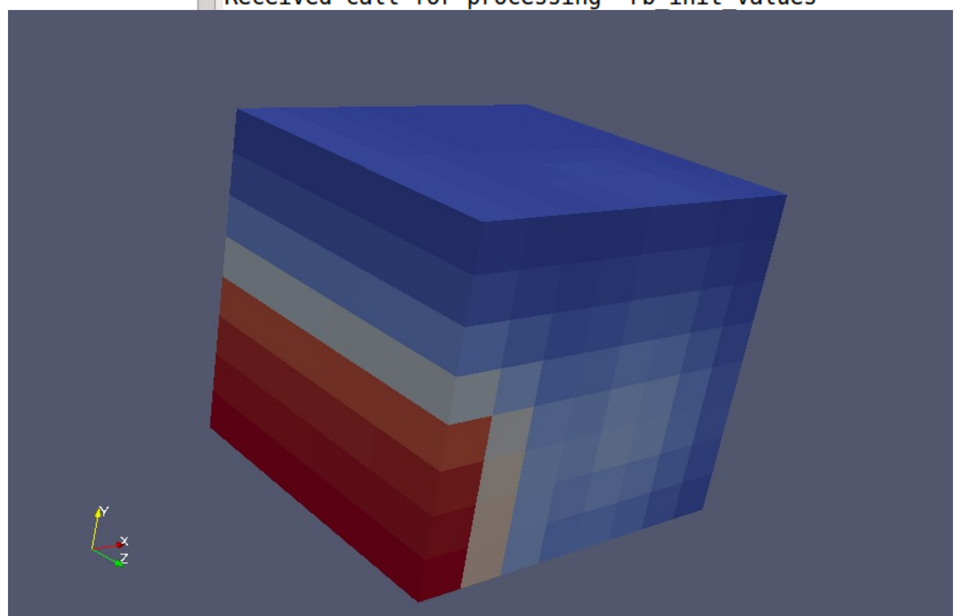
>>
```

```
Received call for processing 'reconstruct_and_compare'
with 2 arguments and 0 return values.
=====================================================

opening file: ./grape//solution.series

Received call for processing 'rb_init_values'
```

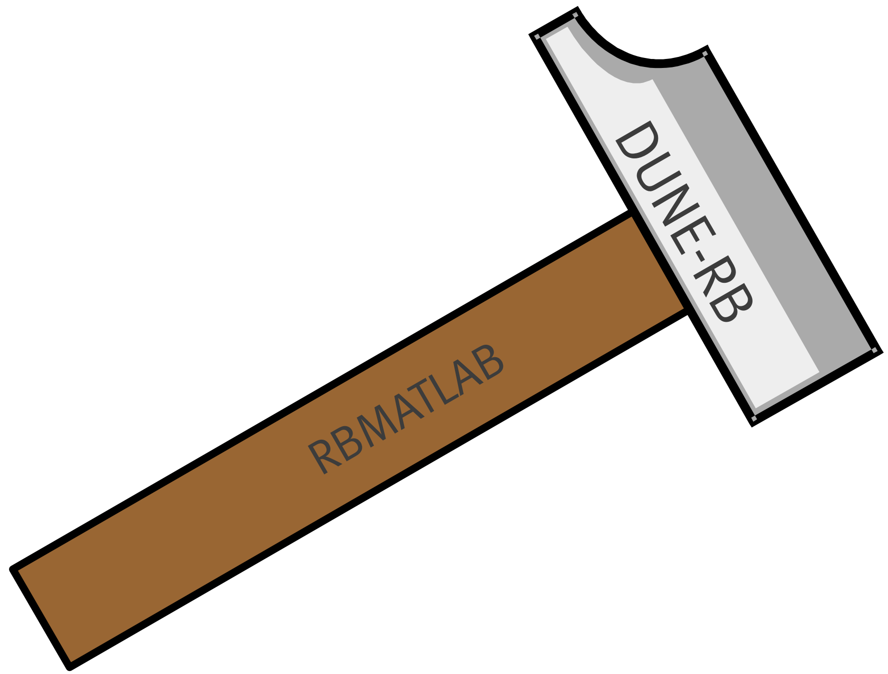


Linear Transport Problem

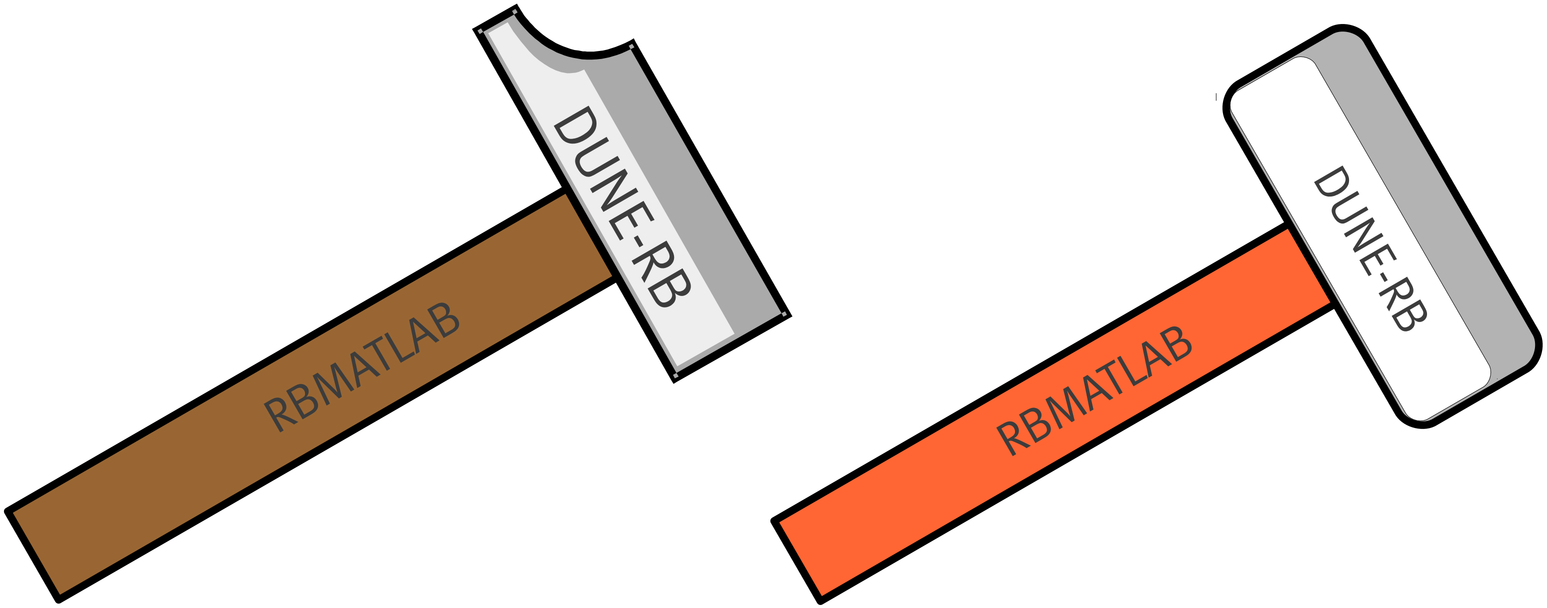
	High-dim. Solution (sec)	RB Generation	Gen. of Online Matrices	Reduced Sim.	Reconstruction	Grid Cells	$L^\infty - L^2$-Error[1]
2D Transport (25 Base Functions)	11	71	6.69	0.11	0.33	1,024	$1.42 \cdot 10^{-3}$
2D Transport (50 Base Functions)	11	2,250	21	0.15	0.42	1,024	$4.64 \cdot 10^{-4}$
3D Transport (50 Base Functions)	944	$1.57 \cdot 10^5$	4,659	0.15	26	32,768	$9.11 \cdot 10^{-4}$

Table 1: Numerical results for a transport problem in 2D and 3D with non-divergence-free velocity.

So, we have a hammer for linear evolution problems ...



… and even one for non-linear problems …



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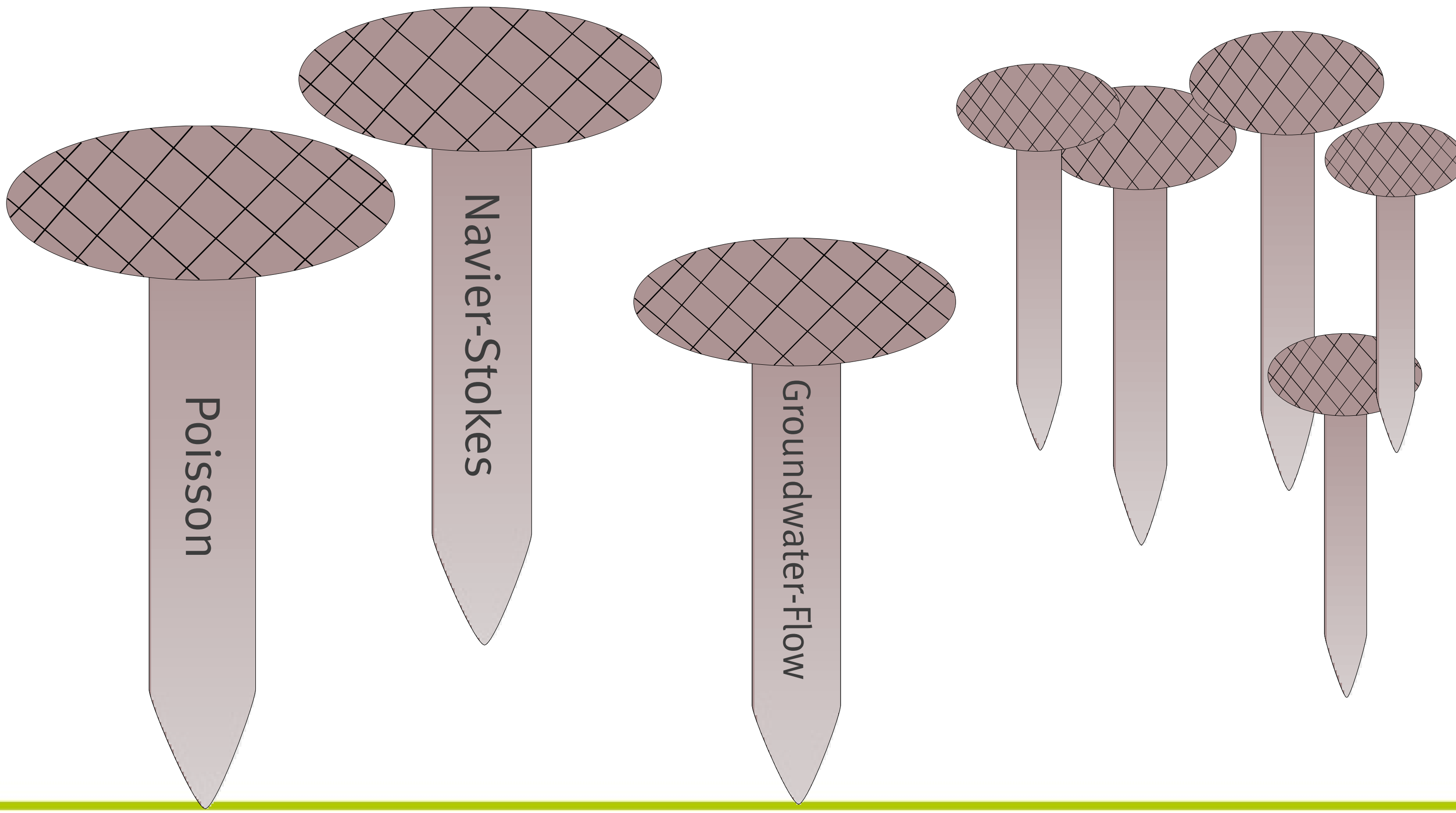
But how do you make your problems look like a nail?



Interface to PDE descretizations

```
>> % Generate the reduced basis with the POD-Greedy algorithm
>> % in DUNE-RB >>>>>>>>
>>
>> detailed_data = gen_detailed_data(model, model_data);
Starting RB extension loop

Detected maximum error prediction 0.044006 for mu=[0.001
    1         0.5]
Extended RB to length 2

Detected maximum error prediction 0.015456 for mu=[0   1   1]
Extended RB to length 3

Detected maximum error prediction 0.012877 for mu=[0
1         0.5]
Extended RB to length 4

Detected maximum error prediction 0.01064 for mu=[0            1
         0.5]
Extended RB to length 5

Detected maximum error prediction 0.0084073 for mu=[0.001
   0.5          1]
Extended RB to length 6

Detected maximum error prediction 0.0073233 for mu=[0   1   1]
Extended RB to length 7

Detected maximum error prediction 0.0055443 for mu=[0   1   1]
Extended RB to length 8

Detected maximum error prediction 0.0048443 for mu=[0
 1         0.5]
```

```
Received call for processing 'rb_operators'
with 2 arguments and 1 return values.
=====================================================


Received call for processing 'get_mu'
with 1 arguments and 1 return values.
=====================================================


Received call for processing 'set_mu'
with 2 arguments and 0 return values.
=====================================================


Received call for processing 'rb_extension_PCA'
with 3 arguments and 1 return values.
=====================================================

opening file: ./grape//solution.series

Received call for processing 'set_mu'
with 2 arguments and 0 return values.
=====================================================


Received call for processing 'rb_init_values'
with 2 arguments and 1 return values.
=====================================================
```

Interface to PDE discretizations (linear)

- For PDE discretization of form

For $\boldsymbol{\mu} \in \mathcal{P}$ compute $\left\{u_h^k(\boldsymbol{\mu})\right\}_{k=0}^{K} \subset \mathcal{W}_h \subset L^2(\Omega)$ by

$$u_h^0(\boldsymbol{\mu}) := P[u_0(\boldsymbol{\mu})]$$

$$u_h^k(\boldsymbol{\mu}) - \Delta t \mathcal{L}^I(\boldsymbol{\mu})[u_h^k(\boldsymbol{\mu})] := u_h^{k-1}(\boldsymbol{\mu}) + \Delta t \mathcal{L}^E(\boldsymbol{\mu})[u_h^{k-1}(\boldsymbol{\mu})].$$

- Implement affinely parameter dependent operators

$$\mathcal{L} = \sum_{q=1}^{Q_L} \boxed{\sigma_L^q(\boldsymbol{\mu})} \, \boxed{\mathcal{L}^q}$$

Interface to PDE discretizations (linear)

Affinely parametrized operators

$$\mathcal{L} = \sum_{q=1}^{Q_L} \boxed{\sigma_L^q(\mu)}\, \boxed{\mathcal{L}^q}$$

with methods

- Parametrization [`set_mu()`]
- Parameter dependent coefficients [`coefficient()`]
- Parameter independent operators [`component()`]

Interface to PDE discretizations (linear)

Affinely parametrized operators

$$\mathcal{L} = \sum_{q=1}^{Q_L} \boxed{\sigma_L^q(\mu)}\, \boxed{\mathcal{L}^q}$$

with methods

- Parametrization [`set_mu()`]
- Parameter dependent coefficients [`coefficient()`]
- Parameter independent operators [`component()`]

⇨ Automatic generation of reduced matrices:

$$(\mathbf{L}^q)_{n,m} = \int_\Omega \mathcal{L}^q [\varphi_m]\, \varphi_n, \qquad q = 1, \ldots, Q_L, m, n = 1, \ldots, N$$

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Interface to PDE discretizations (non-linear)

- For PDE discretizations of the form

For $\boldsymbol{\mu} \in \mathcal{P}$ find $\{u_h\}_{k=0}^K \subset \mathcal{W}_h \subset L^2(\Omega)$, s.t.

$$u_h^0 := P_h\left[u_0(\boldsymbol{\mu})\right], \qquad u_h^{k+1} := u_h^{k+1,\nu_{\max}(k)}$$

with Newton iteration

$$u_h^{k+1,0} := u_h^k, \qquad u_h^{k+1,\nu+1} := u_h^{k+1,\nu} + \delta_h^{k+1,\nu+1},$$

$$\left(\mathrm{Id} + \Delta t \mathbf{D}\mathcal{L}_h^I\big|_{u_h^{k+1,\nu}}\right)\left[\delta_h^{k+1,\nu+1}\right] = u_h^k - u_h^{k+1,\nu} - \Delta t\left(\mathcal{L}_h^I\left[u_h^{k+1,\nu}\right] + \mathcal{L}_h^E\left[u_h^k\right]\right).$$

- Implement empirical interpolation for discrete operators

$$\mathcal{L}_h(\boldsymbol{\mu})\left[u_h^k(\boldsymbol{\mu})\right] \approx \mathcal{I}_M\left[\mathcal{L}_h(\boldsymbol{\mu})\right]\left[u_h^k(\boldsymbol{\mu})\right] = \sum_{m=1}^M l_m(\boldsymbol{\mu})\left[u_h^k(\boldsymbol{\mu})\right] \xi_m$$

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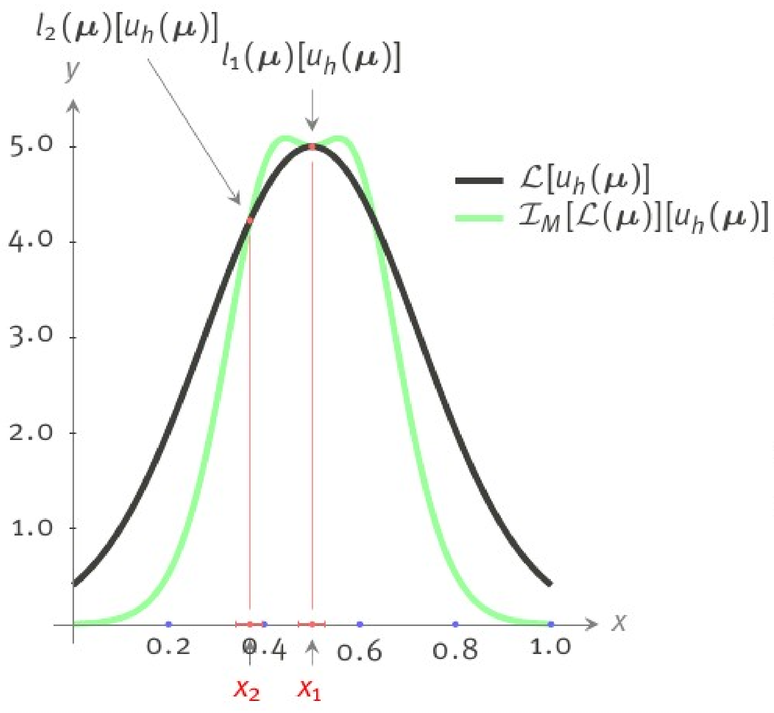
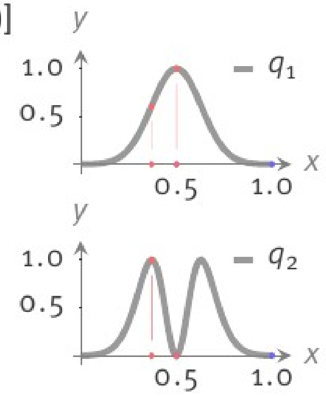
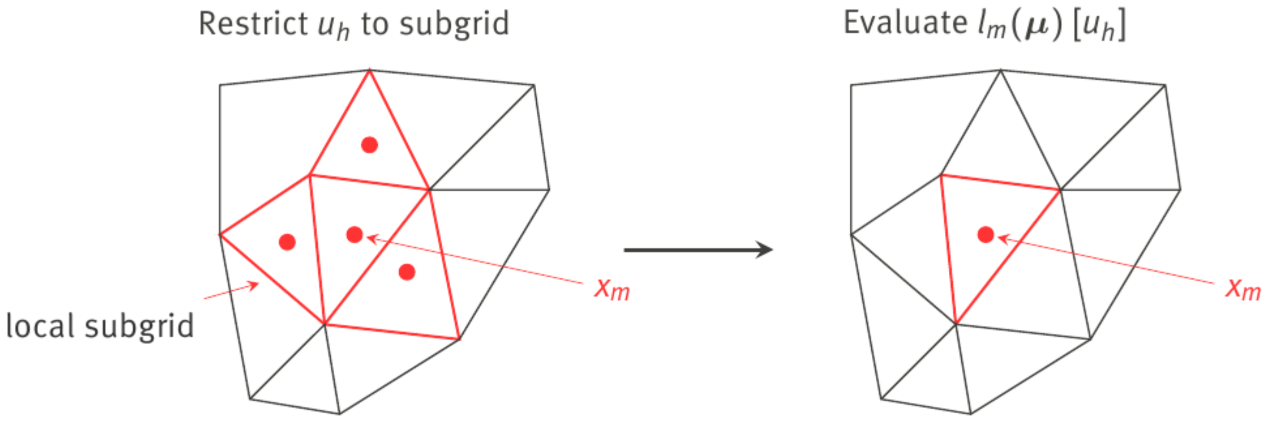
The coefficient functionals $l_m(\boldsymbol{\mu}) = \mathcal{L}_h(\boldsymbol{\mu})[\cdot](x_m)$ can be computed efficiently, if

- Operator has localized structure (small stencil) and
- Local geometry information can be precomputed in offline phase.





Empirical Interpolation for Operators (local grid)



Automatic generation of localized operators

Usual dependencies for local operator evaluations:

$$l_m(\mu) = \mathcal{L}_h(\mu)[\cdot](x_m)$$

Basis function evaluations at quadrature points

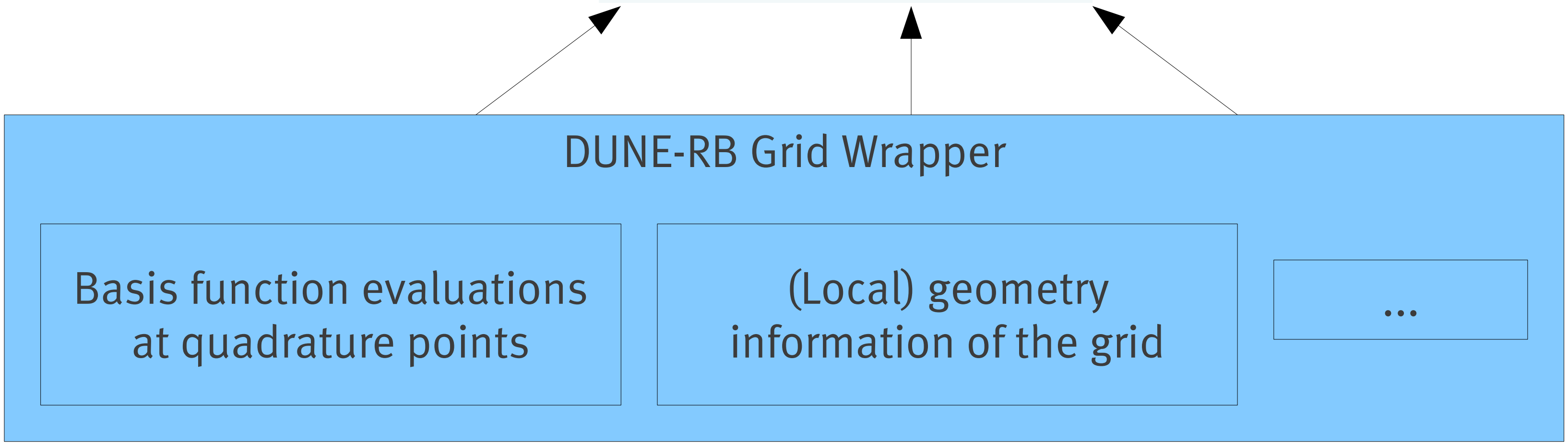
(Local) geometry information of the grid

...

Automatic generation of localized operators

Therefore: Delegation of function calls concerning grid geometry and discrete function space to a wrapper:

$$l_m(\boldsymbol{\mu}) = \mathcal{L}_h(\boldsymbol{\mu})[\cdot](x_m)$$



Behaviour of DUNE-RB Grid Wrapper

- During detailed simulation:

  Delegate calls directly to the grid and the discrete function space

- During offline phase:

  store all grid and discrete function space information concerning the subgrid in low-dimensional data structures

- During online phase:

  Delegate calls to low-dimensional data structures

Conclusion

- Generic implementation of reduced base tools for linear problems is possible
- Empirical interpolation for non-linear problems can be realized with subgrid extraction
- Future work:
  - More examples
  - Tarball – Release with installation instructions is planned, and will be published on http://morepas.org.

Thank you for your attention!